THEOCHEM, VOLUME 47(1988)

(Journal of Molecular Structure, Vol. 170)

AUTHOR INDEX

Arenas, J. F. 233

Bartha, F. 59
Barzaghi, M. 69
Bertrán, J. 225
Biskupič, S. 27
Bogár, F. 59

Carbó, M. 171
Chang, T.-Y. 121
Colwell, S. M. 197
Csizmadia, I. G. 75,107
Czerminski, R. 245

Dovesi, R. 19

Fueno, T. 143

Gamba, A. 69
Gau, Y.-F. 121

Handy, N. C. 197

Ivanov, P. M. 257

Jäger, J. 181
Jen, S.-F. 121
José, J. 171

Kapuy, E. 59
Klein, R. 27
Komasa, J. 205
Kovach, I. M. 159
Kozioł, J. 205
Kozmutza, C. 59
Krechl, J. 239
Kuthan, J. 239

Lee, T.-S. 121
Lien, M. H. 121
Lluch, J. M. 225
Lukovits, I. 249
Luzhkov, V. B. 33

Maksić, Z. B. 39
Manaut, F. 171
Martin, P. S. 107
Mayer, I. 1,9
Morosi, G. 69

Ohsaku, M. 95
Oliva, A. 225
Ou, M.-C. 121

Panas, I. 151
Papadopoulos, M. G. 189
Peterson, M. R. 75
Pipek, J. 213
Poirier, R. A. 1
Pojarlieff, I. G. 257

Quirante, J. J. 233

Ramirez, F. J. 233
Ruckpaul, K. 181
Rychlewski, J. 205

Sanz, F. 171
Schüle, J. 151,155
Schwarze, W. 181
Segura, J. 171
Shainyan, B. A. 133
Siegbahn, P. 151
Silvi, B. 19
Sodupe, M. 225
Strautmanis, J. R. 75
Surján, P. R. 1

Torre, de la, R. 171
Trézl, L. 213

Vetter, R. 85
Vibók, Á. 9

Wahlgren, U. 151
Waite, J. 189
Wu, H.-F. 121
Wünsch, E. 225

Yates, K. 107

Zülicke, L. 85
Zyubin,. A. S. 33

THEOCHEM, VOLUME 47(1988)

(*Journal of Molecular Structure, Vol. 170*)

SUBJECT INDEX

Acetaldehyde,
an attempt to examine alternative MNDO reaction courses of the hydrogen transfer from NADH model to acetaldehyde 239
Activation,
theoretical studies of the activation of C–H and C–C bonds 155
Activation barrier,
MRD-CI study of potential wells and activation barrier of the S_N2 reaction $H^- + CH_3F \rightarrow CH_4 + F^-$ 85
Adiabatic proton transfer,
a theoretical study of adiabatic proton transfer to allene in its ground and excited states 107
Allene,
a theoretical study of adiabatic proton transfer to allene in its ground and excited states 107
Alloxazine,
electronic structure of alloxazine and its methyl derivatives 205

Bromine atoms,
theoretical study of the addition of bromine atoms to monosubstituted and disubstituted derivatives of ethylene 225

C–H and C–C bonds,
theoretical studies of the activation of C–H and C–C bonds 155
Caffeine metabolism inhibitors,
automatic determination of MEP patterns of molecules and its application to caffeine metabolism inhibitors 171
Claverie's method,
reparametrization of Claverie's method for intermolecular energy calculation 245
Conformational structure,
the conformational structure of 1,2-dimethoxyethane in the gas phase 69
Core pseudopotentials,
periodic Hartree–Fock calculations involving core pseudopotentials 19
Cycloaddition reaction,
theoretical study of the symmetry forbidden concerted ethene–ethene cation radical cycloaddition reaction 121
β-Cyclodextrin,
theorectical investigation of inclusion complexes of β-cyclodextrin with alcohols 249
Cytochrome P-450 LM2,
structure–activity relationships on cytochrome P-450 LM2 181

Diastereoisomers,
molecular mechanics of diastereoisomers with phenyl groups on neighbouring carbon atoms 257
Dichlorovinylsulphones,
theoretical study of the mechanism of halogenotropic rearrangement in dichlorovinylsulphones 133
1,2-Dimethoxyethane,
the conformational structure of 1,2-dimethoxyethane in the gas phase 69

Energy derivatives,
second quantization and the Hellmann–Feynman theorem: a unified view on energy derivatives 1
Ethene–ethene cation radical,
theoretical study of the symmetry forbidden concerted ethene–ethene cation radical cycloaddition reaction 121
Ethylene,
theoretical study of the addition of bromine atoms to monosubstituted and disubstituted derivatives of ethylene 225
Ethylnitrene,
intramolecular hydrogen abstraction and

insertion of singlet ethylnitrene 143

Formaldehyde,
formation of excited formaldehyde in model reactions simulating real biological systems 213
Formaldonitrone,
properties of C- and O-protonated formaldonitrone 75

Halogenotropic rearrangement,
theoretical study of the mechanism of halogenotropic rearrangement in dichlorovinylsulphones 133
Hartree–Fock calculations,
periodic Hartree–Fock calculations involving core pseudopotentials 19
Hellmann–Feynman theorem,
second quantization and the Hellmann–Feynman theorem: a unified view on energy derivatives 1
1,5-Hexadienes,
a theoretical approach to the investigation of the photochemical internal cycloaddition: some substituted 1,5-hexadienes 95
Hydrocarbons,
the study of normal saturated hydrocarbons in the localized representation of the MBPT 59
Hydrogen abstraction and insertion,
intramolecular hydrogen abstraction and insertion of singlet ethylnitrene 143
Hydrogen transfer,
an attempt to examine alternative MNDO reaction courses of the hydrogen transfer from NADH model to acetaldehyde 239
Hyperpolarisability,
the polarisability and second hyperpolarisability of some biomolecules 189

Inclusion complexes,
theoretical investigation of inclusion complexes of β-cyclodextrin with alcohols 249
Intermolecular energy,
reparametrization of Claverie's method for intermolecular energy calculation 245

MBPT,
the study of normal saturated hydrocarbons in the localized representation of the MBPT 59
MC SCF study,
MC SCF study of potential curves of small radicals 27
MEP patterns,
automatic determination of MEP patterns of molecules and its application to caffeine metabolism inhibitors 171
Methyl adsorption,
ab initio investigation of methyl adsorption of Ni(111) 151
Microcomputers,
ab initio quantum chemistry on microcomputers 197
MINDO/3 study,
MINDO/3 study of the thermolysis of vinylene carbonate 233
MNDO reaction courses,
an attempt to examine alternative MNDO reaction courses of the hydrogen transfer from NADH model to acetaldehyde 239
MO calculations,
ab initio MO calculations of molecular structure and reactivity of the phenoxy radical 33
Modified atoms,
modified atoms in molecules 39
Molecular mechanics,
molecular mechanics of diastereoisomers with phenyl groups on neighbouring carbon atoms 257
Molecular modeling,
serine hydrolase–phosphyl ester interactions: molecular modeling 159
MRD-CI study,
MRD-CI study of potential wells and activation barrier of the S_N2 reaction $H^- + CH_3F \rightarrow CH_4 + F^-$ 85

NADH model,
an attempt to examine alternative MNDO reaction courses of the hydrogen transfer from NADH model to acetaldehyde 239
Ni(111),
ab initio investigation of methyl adsorption of Ni(111) 151

Phenoxy radical,
ab initio MO calculations of molecular structure and reactivity of the phenoxy radical 33

Photochemical internal cycloaddition,
a theoretical approach to the investigation of the photochemical internal cycloaddition: some substituted 1,5-hexadienes 95
Polarisability,
the polarisability and second hyperpolarisability of some biomolecules 189
Potential curves,
MC SCF study of potential curves of small radicals 27
Potential wells,
MRD-CI study of potential wells and activation barrier of the S_N2 reaction $H^- + CH_3F \rightarrow CH_4 + F^-$ 85

SCF theory,
intermolecular SCF theory with BSSE: the equations and some applications for small systems 9
Second quantization,
second quantization and the Hellmann-Feynman theorem: a unified view on energy derivatives 1
Serine hydrolase-phosphyl ester interactions,
serine hydrolase-phosphyl ester interactions: molecular modeling 159
Structure-activity relationships,
structure-activity relationships on cytochrome P-450 LM2 181

Thermolysis,
MINDO/3 study of the thermolysis of vinylene carbonate 233

Vinylene carbonate,
MINDO/3 study of the thermolysis of vinylene carbonate 233

CONTENTS

Second quantization and the Hellmann–Feynman theorem: a unified view on energy derivatives
P.R. Surján, I. Mayer (Budapest, Hungary) and R.A. Poirier (St. John's, Newfoundland, Canada) 1

Intermolecular SCF theory without BSSE: the equations and some applications for small systems
Á. Vibók (Debrecen, Hungary) and I. Mayer (Budapest, Hungary) 9

Periodic Hartree–Fock calculations involving core pseudopotentials
B. Silvi and R. Dovesi (Paris, France) 19

MC SCF study of potential curves of small radicals
S. Biskupič and R. Klein (Bratislava, Czechoslovakia) 27

Ab initio MO calculations of molecular structure and reactivity of the phenoxy radical
V.B. Luzhkov and A.S. Zyubin (Chernogolovka, Moscow Region, U.S.S.R.) 33

Modified atoms in molecules
Z.B. Maksić (Zagreb, Yugoslavia) 39

The study of normal saturated hydrocarbons in the localized representation of the MBPT
E. Kapuy, F. Bartha (Szeged, Hungary), C. Kozmutza (Budapest, Hungary) and F. Bogár (Szeged, Hungary) 59

The conformational structure of 1,2-dimethoxyethane in the gas phase
M. Barzaghi, A. Gamba and G. Morosi (Milan, Italy) 69

Properties of C- and O-protonated formaldonitrone
J.R. Strautmanis, M.R. Peterson and I.G. Csizmadia (Toronto, Ontario, Canada) 75

MRD-CI study of potential wells and activation barrier of the S_N2 reaction $H^- + CH_3F \rightarrow CH_4 + F^-$
R. Vetter and L. Zülicke (Berlin, G.D.R.) 85

A theoretical approach to the investigation of the photochemical internal cycloaddition: some substituted 1,5-hexadienes
M. Ohsaku (Hiroshima, Japan) 95

A theoretical study of adiabatic proton transfer to allene in its ground and excited states
P.S. Martin, K. Yates and I.G. Csizmadia (Toronto, Ontario, Canada) 107

Theoretical study of the symmetry forbidden concerted ethene–ethene cation radical cycloaddition reaction
T.-S. Lee, M.H. Lien, S.-F. Jen, M.-C. Ou, H.-F. Wu, Y.-F. Gau and T.-Y. Chang (Taichung, Taiwan) 121

Theoretical study of the mechanism of halogenotropic rearrangement in dichlorovinylsulphones
B.A. Shainyan (Irkutsk, U.S.S.R.) 133

Intramolecular hydrogen abstraction and insertion of singlet ethylnitrene
T. Fueno (Osaka, Japan) 143

Ab initio investigation of methyl adsorption on Ni(111)
J. Schüle, I. Panas, P. Siegbahn and U. Wahlgren (Stockholm, Sweden) 151

Theoretical studies of the activation of C–H and C–C bonds
J. Schüle (Stockholm, Sweden) 155

Serine hydrolase–phosphyl ester interactions: molecular modeling
I.M. Kovach (Lawrence, KS, U.S.A.) 159

Automatic determination of MEP patterns of molecules and its application to caffeine metabolism inhibitors
F. Sanz, F. Manaut, J. José, J. Segura, M. Carbó, and R. de la Torre (Barcelona, Spain) 171

Structure–activity relationships on cytochrome P-450 LM2
J. Jäger, W. Schwarze and K. Ruckpaul (Berlin-Buch, G.D.R.) 181

The polarisability and second hyperpolarisability of some biomolecules
M.G. Papadopoulos and J. Waite (Athens, Greece) 189
Ab initio quantum chemistry on microcomputers
S.M. Colwell and N.C. Handy (Cambridge, Gt. Britain) 197
Electronic structure of alloxazine and its methyl derivatives
J. Komasa, J. Rychlewski and J. Kozioł (Poznań, Poland) 205
Formation of excited formaldehyde in model reactions simulating real biological systems
L. Trézl and J. Pipek (Budapest, Hungary) 213
Theoretical study of the addition of bromine atoms to monosubstituted and disubstituted derivatives of ethylene
E. Wünsch, M. Sodupe, J.M. Lluch, A. Oliva and J. Bertrán (Barcelona, Spain) 225
MINDO/3 study of the thermolysis of vinylene carbonate
J.J. Quirante, J.F. Arenas and F.J. Ramirez (Málaga, Spain) 233
An attempt to examine alternative MNDO reaction courses of the hydrogen transfer from NADH model to acetaldehyde
J. Krechl and J. Kuthan (Prague, Czechoslovakia) 239
Reparametrization of Claverie's method for intermolecular energy calculation
R. Czerminski (Warsaw, Poland) 245
Theoretical investigation of inclusion complexes of β-cyclodextrin with alcohols
I. Lukovits (Budapest, Hungary) 249
Molecular mechanics of diastereoisomers with phenyl groups on neighbouring carbon atoms
P.M. Ivanov and I.G. Pojarlieff (Sofia, Bulgaria) 257

Author index 269

Subject index 270